

crystallographic symmetry (NCS) averaging (if required) and partial/complete model building. Once important parameters are entered, X-ray derivative data are loaded and the process is invoked by pressing the „submit“ button, no further user intervention is needed. The GUI allows the users to follow the progress and provides a tarball of the initial model, electron density, bones and a macro for O/COOT/XFIT to view the model and map on appropriate computer graphics. The platform has been installed on a Linux cluster at EMBL-Hamburg and is remotely accessible to the beamline users via a web-server. The server [2] is accessible from most Internet browsers and allows beamline users and the crystallographic community to validate their X-ray diffraction experiments in the shortest possible time. An overview of *Auto-Rickshaw* with its architecture, functionality, some examples and the way this platform is used as a feedback system for X-ray data collection or validation of the X-ray experiment, will be discussed.

[1] Panjikar S., Parthasarathy V., Lamzin V.S., Weiss M. S. & Tucker, P.A. **2005**. *Acta Cryst.* D61, 449-457. [2] <http://www.embl-hamburg.de/Auto-Rickshaw/>

**Keywords: automation; phasing; remote access for crystallography**

#### FA5-MS03-O4

**Automation and Remote Access on the ESRF's Macromolecular Crystallography Beamlines.** Leonard Gordon. *Macromolecular Crystallography Group, European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38043 Grenoble Cedex, France.*

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The end-stations dedicated to Macromolecular Crystallography (MX) at the European Synchrotron Radiation Facility (ESRF) currently welcome over 2600 visitors each year with experimental sessions lasting anything from 4 hours to 2 days. To cope with such a high user throughput and to ensure the beam-lines are reliable and user-friendly, the MX Group at the ESRF has developed a policy of, where possible, standardising hardware and software in both optics and experimental hutches of the beam-lines. Such standardisation, and the fact that MX 'experiments' are essentially repetitive in nature, lends itself to automation. The automation available on the ESRF's MX beam-lines [1-6] will be described.

For several years, a form of remote access to the ESRF's MX beam-lines has been available to industrial users via the highly successful MxPress data collection service. However, manpower requirements mean that a similar service cannot be offered to academic users. We have therefore, as a direct result of the high levels of automation now in place, developed a system, accessible to industrial and academic users alike, whereby experimenters can control the ESRF's MX beamlines from the comfort of their home laboratories [7]. The remote access protocols used at the ESRF will also be described as will our experiences, both good and bad, with the system currently deployed.

[1] Arzt *et al.*, **2005** *Prog. Biophys. and Mol. Biol.*, 89, 124-152. [2] Cipriani *et al.*, **2006**. *Acta Cryst.*, D62, 1251-1259. [3] Beteva *et al.*, **2006**. *Acta Cryst.*, D62, 1162-1169. [4] Leslie *et al.*, **2002**. *Acta Cryst.*, D58, 1924-1928. [5] Giraud *et al.*, **2009** *J. Appl. Cryst.*, 42, 125-128. [6] Leonard *et al.*, **2009** *J. Appl. Cryst.*, 42, 333-335 [7] Gabadinho *et al.*, **2008** *Synchrotron Radiation News*, 21, 24-29.



Academic users controlling their experiment at an ESRF MX beam-line from their offices at the University of York, UK

**Keywords: automation; remote access; synchrotron facilities**

#### FA5-MS03-O5

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The process of determining macromolecular crystal structures may be thought of as a simple sequence of operations: protein production, crystallization, diffraction, phasing, model building, refinement and deposition of coordinates. This sequence is sufficiently understood and all steps of such pipeline may be automated. The yield of the structure determination pipeline depends on many organizational and human factors. One of the ways to speed up this process is to facilitate access to a few synchrotron radiation centers operating worldwide. Beamlines on these facilities have long queues, and increasing the efficiency of utilization of these facilities will help in expediting the structure determination process. Most of the synchrotron centers offer remote data collection capabilities on its macromolecular beamlines. Remote experimenters have access to the same tools as local users, have the capability to manipulate crystalline samples and to collect, analyze, and backup diffraction data. Automation and remote data collection are therefore essential steps in ensuring that macromolecular structure determination becomes a very high throughput process.

[1] Gilski M., *Acta Phys. Pol. A*, **2008**, 114(2), 331. [2] Jaskolski M., Gilski M., *Academia*, **2007**, 3, 8.

**Keywords: automated data collection; remote access for crystallography; macromolecular synchrotron X-ray crystallography**